

The zeros distribution of Z_5 -symmetric model on a triangular lattice

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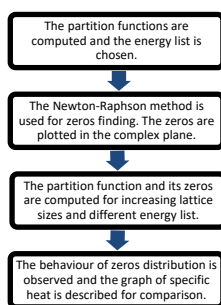
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Graphical abstract



Abstract

We study the Z_Q -symmetric model with the nearest neighbour interaction between molecular dipole of five spin directions i.e. $Q=5$ which called as the Z_5 -symmetric model on a triangular lattice. We investigate the zeros of partition function and the relationship to the phase transition. Initially, the model is defined on a triangular lattice graph with the nearest neighbour interaction. The partition function is then computed using a transfer matrix approach. We analyse the system by computing the zeros of the polynomial partition function using the Newton-Raphson method and then plot the zeros in a complex plane. For this lattice, the result shows that for specific type of energy level there are multiple line curves approaching real axis in the complex plane. The equation of the specific heat is produced and then plotted for comparison. Motivated from the work by Martin (1991) on models on square lattice, we extend the previous study to different lattice type that is triangular lattice.

Keywords: statistical mechanics, Z_Q -symmetric model, partition function, crystal lattice, phase transition, exact result

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INTRODUCTION

The Z_Q -symmetric model [1] is one of the models in statistical mechanics, an area of physics where mathematical modelling is used to investigate physical system [2, 3]. The Z_Q -symmetric model is related to the Q -state Potts model [3] where Q is the number of possible spin orientations. One interesting problem is in modelling a phase transition phenomena [2, 4, 5]. For $Q=2$, this model corresponds to the Ising model [2]. For $Q=3$, this model corresponds to the 3-state Potts model. For the one-dimensional Ising model, Ising [2] showed that it has no phase transition. Later Peierls showed the existence of ferromagnetism in higher dimension at sufficiently low temperature [6]. Then Onsager [7] successfully described the exact solution of the Ising model on square lattice and showed the result related to the phase transition critical point. The models spin directions are presented using discrete numbering but for this research, the model involves angle between 2 variables. Without loss of generality, the angle is represented in discrete numbering with specific model parameters and rescaling factors.

The study of complex-temperature zeros of partition function was first discussed by Fisher [8] for square lattice Ising model and also separately by [9, 10, 11]. The singularity of specific heat, which corresponds to the existence of the phase transition is discussed by observing the arc in the zeros distribution. The zeros of the partition function are studied in order to find the analytic properties of the phase transition in a finite size system [12,13]. The phase transition point is determined from the zeros distribution in a pattern [8] that consists of subsets of set of zeros called locus of zeros.

At the thermodynamic limit for square lattice Ising model, the locus cuts the real axis of the complex plane at the thermodynamic critical point [8, 14]. The zeros will always lay-off the real axis of the complex

plane for a finite system but may very close to the real axis in thermodynamic limit – specifically very close to the critical point of phase transition (for finite lattice we will never find this, but for limiting size approaching infinity case, we may determine this like Onsager's solution). Also, this locus of zeros is supported by a theorem called Lee-Yang theorem where Lee and Yang [15] proved that the zeros of square lattice Ising model must be lie in a unit circle.

The critical point at positive real axis is the exact point where specific heat given by the logarithm of partition function has a singularity. This point is determined by the locus of zeros (as in Fisher's zeros on square lattice Ising model) or by the limiting equation of the largest eigenvalue Ising model matrix [1]. For the zeros distribution of finite lattice, although we cannot directly determine this critical point, as mentioned earlier it will approach the value as the size increases. A locus of point is expected to be observed as we increase the size (need to have specific boundary condition which will give line distribution). Onsager in his square lattice Ising model showed that the phase transition is observed when there is a singularity in the graph of the specific heat [1, 7].

Based on the work by Martin [1] and Zakaria [16] on the Z_Q -symmetric model on a square lattice, they suggested that the emergence of multiple line curves on the complex-temperature plane can also predict the existence of multiple phase transitions. In this study, we extend the study to a different lattice type.

Here, we study for $Q=5$, the Z_5 -symmetric model on triangular lattice in increasing lattice sizes. We study a model of spin variables on graph representing the molecular dipole on a crystal lattice of a physical system.

The outline of this paper is as follows: The basic definition of the graph and the Z_Q -symmetric model are initially presented. The lattice

model Hamiltonian on triangular lattice is introduced with some examples. Then, we compute the partition function on several cases of energy level in increasing lattice sizes. The list of the computed cases is presented in a table. The partition function is then analysed for its complex zeros and we present the result in complex Argand plane. The specific heat equation is computed and plotted for comparison.

Preliminaries

The model consists of discrete variables representing magnetic dipole moments of atomic spins. The spins are placed on a lattice represented by a graph. All vertices of the graph are referring to the spin variables, where they are embedded to the Euclidean space \mathbb{R}^3 . Each spin interacts with its nearest neighbors and the external magnetic field h is assumed to be zero. The graph is defined as below.

Definition 1 [17] A graph Λ is a triple $\Lambda = (V, E, f)$. The V is a set. The elements $v \in V$ are called vertices. The E is also a set. The elements $e \in E$ are called edges. The f is a function $f: E \rightarrow V \times V$. Given $e \in E$ and $v_1, v_2 \in V$, the images $f(e) = \langle v_1, v_2 \rangle$ give the 'source' and 'target' vertex of edge e .

Definition 2 [16] The distance $d(u, v)$ is the number of edges in the shortest path from u to v . Two vertices $u, v \in V$ are called nearest neighbours if $f(e) = \langle v_1, v_2 \rangle$ for some $e \in E$ i.e. when $d(u, v) = 1$.

Definition 3 Consider a set W of lattice sites, each with a set of adjacent sites (nearest neighbours) forming a d -dimensional lattice. For each lattice site $k \in W$ there is a discrete variable σ_k such that $\sigma_k \in \{1, 2, \dots, Q\}$, representing the site's spin. A spin configuration, $\sigma = (\sigma_k)_{k \in W}$ is an assignment of spin value to each lattice site.

For any two adjacent sites $i, j \in W$, $d(i, j) = 1$, there is an interaction strength J . The interaction between two adjacent sites will produce energy called Hamiltonian. The Hamiltonian is one of the physical observables [7, 11] that can be experimentally measured, which represents the total energy of a system.

Similar with the Ising model [4], if $J > 0$, then the system is in a ferromagnetic state. The energy of the system is at the lowest where all spins variables are oriented in the same direction. Conversely, if $J < 0$, then the system is in an antiferromagnetic state, where the orientation of each spin variable is different to its nearest neighbours.

MATHEMATICAL MODEL

The Z_Q -symmetric Model

The Z_Q -symmetric model can be illustrated by the idea of a clock-like circle, for spin directions. The Z_Q in Z_Q -symmetric is referred to the symmetry group that is the discrete rotation group of order Q . The interaction between one spin to another gives an energy value. Due to the arrangement of energy in a clock-like circle – which for literal clock has 12 points marked around the face, this model sometimes called a clock model. The spins take values from Z_Q transformation and the Hamiltonian is invariant under a global Z_Q transformation [1]. The energy difference remains the same when any pair of the spin direction is moved with fixed angle around the clock. This fixed energy difference is then characterised the symmetry of the model [17].

Our model (also known as clock model due to this illustration of energy) categories a different type of energy by a list of energy $\tilde{\chi}$. It is the list of possible choices of energy values written as $\tilde{\chi} = (\tilde{\chi}[0], \tilde{\chi}[1], \tilde{\chi}[2], \dots) \in [0, 1]$, for Q spin directions. We initially assume the energy is positive between $[0, 1]$ and because of the symmetry, we only list half of the different interactions i.e. for $Q=5$, $(\tilde{\chi}[0], \tilde{\chi}[1], \tilde{\chi}[2])$ – we need $Q \times Q$ matrix of values for completely general Q case. The list is arranged by the increasing order of angle relative to 1 spin direction.

Figure 1 shows the examples of the clock interaction of a spin direction relative to another spin denoted as spin 1. Together in the clock, their energy are also described illustratively. The direction is

written inside the clock and the energy is written outside the clock. Here, the energy is written as $(1, \gamma_1, 0)$.

For model (a), the spins are oriented in the same direction whereas for model (b) and (c), the spins are oriented in the different directions in which the spin 1 interacts with the spins 3 and 5, respectively. The energy is written based on the spins interaction relative to spin 1. Due to symmetry, the energy between interactions of spins 1-3 is equal to spin 1-4, and by rotational transformation, is equal to spins 2-4 and spins 3-5. Their energy is 0. In these cases, the spin difference is the same, that is 2.

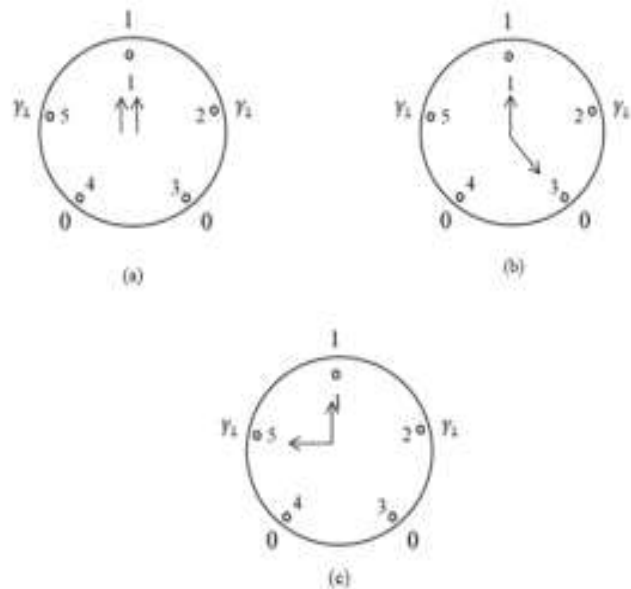


Figure 1 Examples (a, b, and c) of the interaction of a spin relative to spin 1 represented by a pair of arrow.

For 2 spin variables oriented in the same direction, the energy for this nearest neighbour is equal to $\tilde{\chi}[0] = 1$. If it differs by 1 (e.g. for $Q=5$, 1-2, 1-5, 2-3 etc) the energy is $\tilde{\chi}[1]$. Note that by symmetry and the clock circle, for $Q=5$, 1-5 is differed by 1. Similarly, when it differs by 2 (e.g. for $Q=5$, 1-3, 1-4, 2-4 etc) the energy is $\tilde{\chi}[2]$. The energy penalty of $\tilde{\chi}$ is the energy difference between the energy values of two spin configurations, given by $(\tilde{\chi}[0] - \tilde{\chi}[1], \tilde{\chi}[1] - \tilde{\chi}[2], \dots)$ -step. We describe the specific energy penalty and its zeros distribution in the result section.

In general, the Hamiltonian function (defined for energy value between spins) can be written as

$$\mathcal{H}(\sigma) = -J \sum_{\substack{\langle i, j \rangle = f(e), \\ e \in E}} g(\sigma_i, \sigma_j).$$

To ease the computation, the function g is rescaled to discrete value to $g'_r(\sigma_i, \sigma_j) = \gamma_r g_r(\sigma_i, \sigma_j) + \tilde{\gamma}_r$ where $\gamma_r, \tilde{\gamma}_r \in \mathbb{R}$ are the rescaling factors.

We define the Hamiltonian for Z_Q -symmetric model as the following. The value of the Hamiltonian in the equation (2) depends on the angle between two adjacent spins or by the distance of two spin directions. If the angle between two spin directions is small, it will contribute to a lesser energy loss as compared to the large angle. This energy loss is called the energy penalty. The energy is equivalent to the Potts model when the pair of spin variables (σ_i, σ_j) is pointed in the same direction [1, 2]. For the Potts model, the energy value is 1 when two nearest neighbour spins are pointed at the same direction and 0 otherwise.

Definition 4 For any microstate $\sigma \in \Omega$, the Hamiltonian of the Z_Q -symmetric model is defined as,

$$H_\chi(\sigma) = -J \sum_{\substack{(i,j) \in E \\ e \in E}} \chi[\sigma_i - \sigma_j]$$

$$= -J \sum_{\substack{(i,j) \in E \\ e \in E}} \sum_{r=1}^{\lfloor \frac{Q}{2} \rfloor} \gamma_r \cos \left(\frac{2\pi r(\sigma_i - \sigma_j)}{Q} \right) + \tilde{\gamma}_r \quad (2)$$

where $\lfloor \frac{Q}{2} \rfloor$ is the discrete value of the division and $\gamma_r, \tilde{\gamma}_r \in \mathbb{R}$ are model parameters that fixed for a given model.

We remove the quotient value of the Z_Q -symmetric model by rescaling the Hamiltonian function. We introduce a new notation χ by denoting that the energy is in discrete value after the rescaling. Our model is focused on this positive discrete energy list χ assumption (the value is initially chosen from quotient value in range $[0,1]$ and then rescaled into integer value). By this assumption, we study the partition function for different and computable χ .

In a slightly different setting, without the positive assumption, see Example 1. For each interacting pair of spins, the Hamiltonian is calculated and rescaled to get the integer value.

Example 1 Let $Q=5$ and the energy value for each pair of spin variables is represented by **Table 1**. Let $g_r(\sigma_i, \sigma_j) = \cos(2\pi r(\sigma_i - \sigma_j)/Q)$ and $\lfloor Q/2 \rfloor = 2$.

Table 1 The $g_r(\sigma_i, \sigma_j)$ for Z_5 -symmetric model.

σ	1	2	3	4	5
1	2	-1/2	-1/2	-1/2	-1/2
2	-1/2	2	-1/2	-1/2	-1/2
3	-1/2	-1/2	2	-1/2	-1/2
4	-1/2	-1/2	-1/2	2	-1/2
5	-1/2	-1/2	-1/2	-1/2	2

The value of $g_r(\sigma_i, \sigma_j)$ in Table 1 can be rescaled to $g'_r(\sigma_i, \sigma_j) = \gamma_r g_r(\sigma_i, \sigma_j) + \tilde{\gamma}_r = \frac{2}{5} g_r(\sigma_i, \sigma_j) + \frac{1}{5}$. This energy is reduced to the 5-state Potts model shown in **Table 2**.

Table 2 The $g'_r(\sigma_i, \sigma_j)$ for Z_5 -symmetric model.

σ	1	2	3	4	5
1	1	0	0	0	0
2	0	1	0	0	0
3	0	0	1	0	0
4	0	0	0	1	0
5	0	0	0	0	1

Models on triangular lattice

The model is defined on a triangular lattice with the nearest neighbour interaction. The triangular lattice has discrete variables called vertices with associated spin which can take any value of $\{1, 2, \dots, Q\}$ that represents the spin direction. In this paper, we consider $Q = 5$. The lattice site and the interaction of the nearest neighbour are represented by the vertex and the edge of the graph, respectively.

Each lattice site has three successive nearest neighbours. See Figure 2 for illustration. Figure 2 (left) is the triangular lattice 3 by 4 (or 3×4 – 3 row and 4 column vertices). That lattice is then rearranged as in Figure 2 (right) for computing purposes (for transfer matrix approach – will be explained after this).



Figure 2 The 3 by 4 triangular lattices.

Consider a model of n vertices and Ω be the set of all possible configurations;

$\Omega = \{ \sigma(x) = (\sigma_1, \dots, \sigma_n) : \sigma_i = \{1, 2, \dots, Q\}, i \in V, i = 1, \dots, n \}$. See Figure 3(a) for 2 by 2 triangular lattice example. All vertices are labelled by the spin state σ_i .

For arbitrary N by M triangular lattice (refer to Figure 3b), the N corresponds to the number of row vertices while M is the number of column vertices. The dash dot lines and the dot lines are edges that connecting the lower and upper vertices for the triangular shapes – these edges represent the vertical boundary condition.

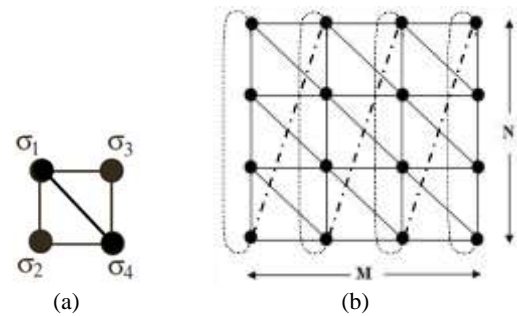


Figure 3 (a) 2 by 2 triangular lattice. (b) Triangular lattice with system size $N \times M = 4 \times 4$.

Partition function and transfer matrix

We study the partition function of Z_5 -symmetric model. The partition function is a function that relates temperature and other parameters with the states of a spin system [3, 5]. We define the partition function as follows.

Definition 5 For a given Q and Λ , the partition function is defined as

$$Z_\Lambda(\beta) = \sum_{\sigma \in \Omega_\Lambda} \exp(-\beta \mathcal{H}_\Lambda(\sigma)) \quad (3)$$

where the summation is over all possible microstates σ of a system, the $\beta = 1 / (k_B T)$ in which k_B is the Boltzmann's constant and T is the absolute temperature.

The partition functions are computed by transfer matrix approach [1, 3, 14] for an increasing finite lattice sizes. The $Z(x)$ is written in a polynomial form by letting $x = e^\beta$.

Definition 6 For a given graph G , the partition vector $Z_G^{V'}$ is the vector arrangement in space of all fixed boundaries or exterior sites, V' of a lattice system. For boundary configuration $\sigma_B \in \Omega_{V'}$, we have

$$Z_G^{V'} = \{ Z_G^{V'} |_{\sigma_1}, Z_G^{V'} |_{\sigma_2}, \dots \},$$

$B=1, 2, \dots$ is referring to the different configurations of the exterior sites.

Then, the full partition function is defined as

$$Z_G = \sum_{\sigma_B \in \Omega_{V'}} Z_G^{V'} |_{\sigma_B}. \quad (4)$$

For two combined lattice graphs, its partition function can be produced by vector arrangement and by combining the two lattices through a vector multiplication – a bigger lattice can be formed (see [1, 3, 14] for details).

Definition 7 Let G, G' be two lattice graphs. For the union of two graphs $G \cup G'$ we have

$$V_{G \cup G'} = V_G \cup V_{G'}$$

$$E_{G \cup G'} = E_G \cup E_{G'}.$$

The E is the set of edges and $E_G \cap E_{G'} = \emptyset$.

A summation of the product of partition vectors for graph G and G' can produce the partition function of the new graph $G \cup G'$ denoted as GG' . Based on the Chapman-Kolmogorov theorem [18], this partition function is given by

$$Z_{GG'} = \sum_{\sigma \in \Omega_{V'}} (Z_G^{V'} |_{\sigma}) (Z_{G'}^{V'} |_{\sigma}) = Z_G^{V'} Z_{G'}^{V'}. \quad (5)$$

Lemma 1 (Chapman-Kolmogorov equation [18]) Let G_1 and G_2 be two graphs such that $E_{G_1} \cap E_{G_2} = \emptyset$. Let $G_1 G_2 = G_1 \cup G_2$ and $V = V_{G_1} \cup V_{G_2}$ and $V' \subseteq V_{G_1 G_2}$. Then

$$Z_{G_1 G_2}^{V'} |_{c'} = \sum_{c \in \Omega_{V'}} (Z_{G_1}^{V'} |_{c', c}) (Z_{G_2}^{V'} |_{c', c}), \quad (6)$$

where c', c is the configuration associated to V' and then to V .

The partition vector $Z_G^{V'}$ is reorganised into a matrix denoted as T which is called a transfer matrix. The incoming and outgoing sites are corresponded by the two columns denoted as V_I and V_O (refer Figure 3(a) for example, where $v_{\sigma_1}, v_{\sigma_2} \in V_I$ and $v_{\sigma_3}, v_{\sigma_4} \in V_O$) respectively such that $V = V_I \cup V_O$. The row and column matrices are representing the set of all possible configuration states Ω_{V_I} and Ω_{V_O} respectively. Each entry in matrix T is given by

$$T_{ij} = Z_G^{V'} |_{\sigma_i \in \Omega_{V_I}, \sigma_j \in \Omega_{V_O}}. \quad (7)$$

By a matrix multiplication, we can combine two graphs that similar to partition vector multiplication. Given T_G and $T_{G'}$ are the transfer matrices associated to graph G and G' and $E_G \cap E_{G'} = \emptyset$, we can use these transfer matrices to combine the graph. The transfer matrix multiplication is given by

$$T_{GG'} = T_G T_{G'}, \quad (8)$$

where the incoming sites of GG' are equal to the incoming sites of G , $V_{I_{GG'}} = V_{I_G}$ and the outgoing sites of GG' are equal to the outgoing sites of G' , $V_{O_{GG'}} = V_{O_{G'}}$.

The new partition function is given by

$$Z_{GG'} = \sum_{i=1}^d \sum_{j=1}^d (T_{GG'})_{i,j}, \quad (9)$$

where i, j is the index of entries in matrix $T_{GG'}$, and d is the dimension of the matrix.

The zeros distribution

The partition function (in polynomial form $x = e^\beta$) is analysed by implementing the computational method of zeros finding, by setting $Z = 0$.

The model's partition function is a positive polynomial. Hence, the zeros must have at least 1 complex plot. Additionally, its complex conjugate is also the root of the polynomial. The Newton-Raphson method is used in finding the zeros of the partition function. A C++ programming language is used for the computation (with the Gnu multiple precision library as another essential tool). All the zeros are plotted in the complex Argand plane.

RESULTS AND DISCUSSION

We write $N \times M'$ for N number of row vertices and M number of column vertices. The prime in M' corresponds to the open boundary condition. The number without prime corresponds to the periodic boundary condition.

We study the model on triangular lattice with periodic boundary condition in vertical direction and open boundary condition in horizontal direction.

The zeros of partition function are plotted in complex-temperature Argand plane. Due to the limitation of computing resources (due to Moore's law), only several small lattice sizes are manageable to be computed. Although the phase transition occurs at the thermodynamic limit when the system is approaching limit – very big in size and huge number of vertices, the behaviour of limiting cases can already be observed in a small discrete cases. Due to this reason, we try to extract as much as possible information from our computable cases relating to the phase transition. Following the square lattice case [14], we observe the pattern of zeros in the physical region (all areas of plane bounded by real part $x > 0$).

The zeros are computed for $x = e^\beta$. This plot shows that the positive real axis is the only range that has a physical meaning. For ferromagnetic case $J > 0$, the physical region is given by the region enclosed by real part $[1, \infty)$ – this region is the ferromagnetic region and the rest is unphysical. For the antiferromagnetic case $J < 0$, the region enclosed by real part $[0, 1]$ is the antiferromagnetic region and the rest is unphysical. Modeling the zeros distribution of a physical system gives us the information for two different systems of magnetism – ferromagnetic and antiferromagnetic systems. The critical point of the phase transition is a real-valued constant exactly on the real line of the distribution. For the finite case, the zeros will never actually cross this real line (we need very big lattice to at least have the root very close to the real axis, or the thermodynamic limit for the cross-over point). But the locus of zeros for example as plotted for the Onsager solution [7] by Fisher in [8] gives this critical point – the locus is a circle center at $(1, 0)$ and radius $\sqrt{2}$. The point where the locus of zeros cuts the real axis is the critical point of the phase transition.

The lists of results of the zeros distribution of the partition function for Z_5 -symmetric model are written in Table 3. We compute the zeros distribution for several cases of the energy χ for increasing lattice sizes. We present some of the zeros distributions to highlight our finding related to the phase transition properties.

The number of linear arc is observed for the zeros near the real axis in the physical region. The claim is that the single arc corresponds to the single phase transition while the multiple arcs correspond to the multiple phase transitions.

Table 3 The zeros distribution computed cases for Z_5 -symmetric model with arbitrary energy list χ .

	χ	$5 \times 5'$	$6 \times 6'$	$7 \times 7'$	$8 \times 8'$	$9 \times 9'$
$Q = 5$	(2,1,0)					
	(3,1,0)					
	(3,2,0)					
	(4,1,0)					
	(4,3,0)					
	(5,1,0)					
	(5,3,0)					
	(5,4,0)					
	(6,1,0)					
	(6,5,0)					

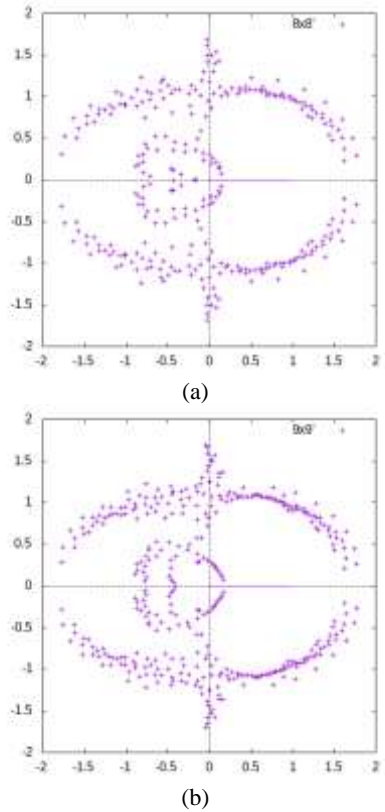


Figure 4 Zeros distribution for $\chi = (2,1,0)$; a) $N=8$, b) $N=9$.

See Figure 4 for $\chi = (2,1,0)$. We observed that the zeros form a single curve towards the positive real axis. As the lattice size increases, the appearance of the curves becomes clearer. In the ferromagnetic region when $\chi > 1$, there are multiple arcs that move closer to the real axis as the lattice size increases. But it is still not clear enough either the arcs will remain or merge into single line since we need bigger lattice size to determine it.

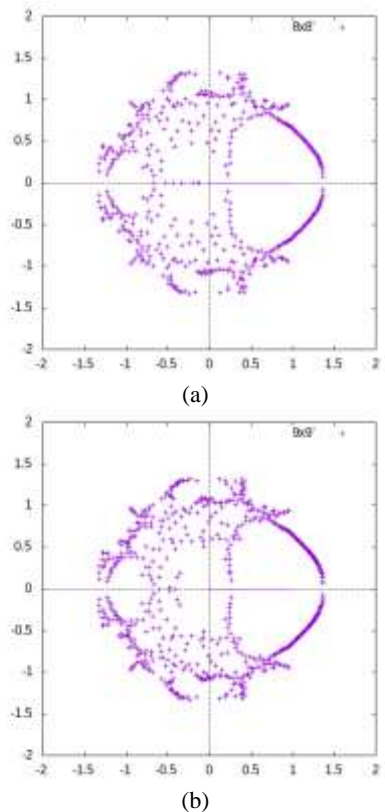


Figure 5 Zeros distribution for $\chi = (3,1,0)$; a) $N=8$, b) $N=9$.

Figure 5 shows the zeros distribution for $\chi = (3,1,0)$. As the lattice size increases, a single line of zeros approaches the real axis in the ferromagnetic region. In the antiferromagnetic region, a linear arc is formed at 9×9 case that is close to the real axis. This single line suggests the existence of single phase transition.

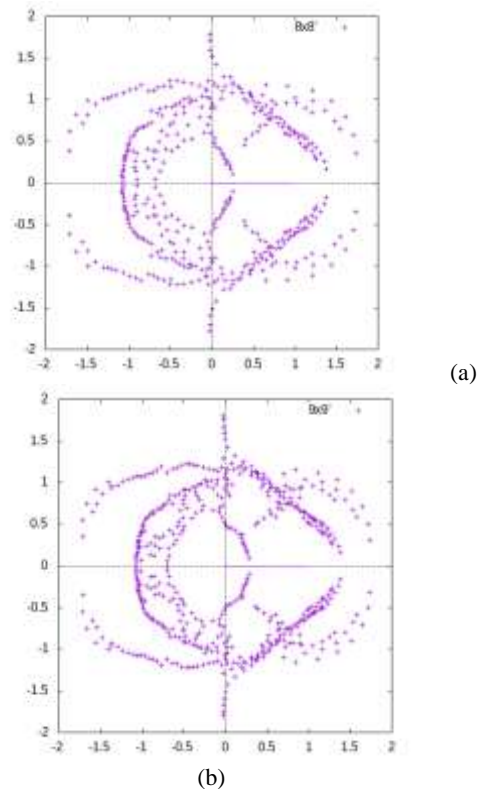


Figure 6 Zeros distribution for $\chi = (3,2,0)$; a) $N=8$, b) $N=9$.

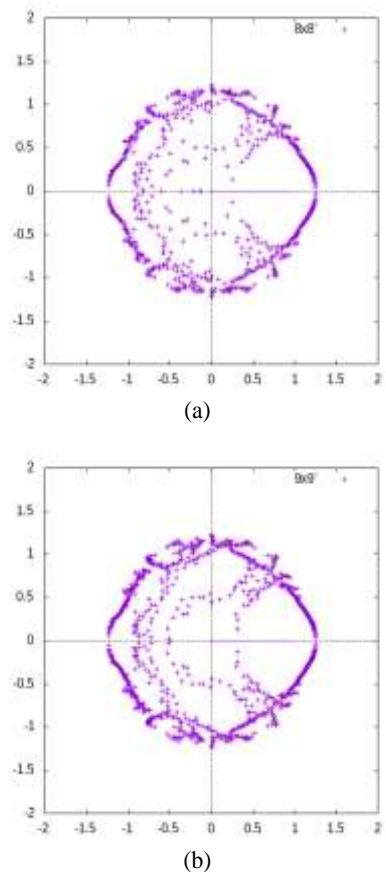


Figure 7 Zeros distribution for $\chi = (4,1,0)$; a) $N=8$, b) $N=9$.

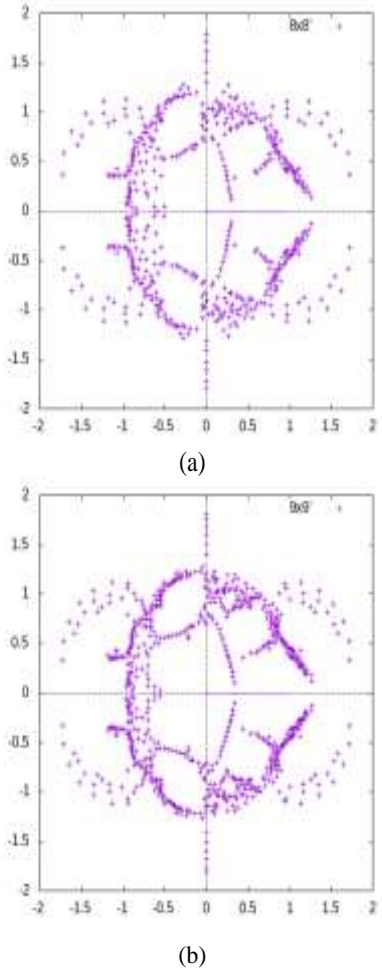


Figure 8 Zeros distribution for $\chi = (4, 3, 0)$; a) $N=8$, b) $N=9$.

For $\chi = (3, 2, 0)$ in Figure 6, the zeros distribution obviously shows the existence of two arcs in the positive real axis. As the lattice size increases, the lines become clearer. A single curve also moves closer towards the real axis in the antiferromagnetic region. In the non-physical region, there is an arc approaching the real axis.

We make further comparison for the zeros distribution based on its energy penalty effect. The $\chi = (3, 1, 0)$ has (2,1)-step energy penalty and the $\chi = (3, 2, 0)$ has (1,2)-step energy penalty. The case $\chi = (3, 1, 0)$ in Figure 5 shows the existence of single line in the ferromagnetic region. Interestingly for $\chi = (3, 2, 0)$ in Figure 6, the distribution in ferromagnetic region shows multiple lines approaching the real axis.

Similarly, we present the distribution of zeros for $\chi = (4, 1, 0)$ and $\chi = (4, 3, 0)$ with their energy penalty as seen in Figure 7 and 8. The $\chi = (4, 1, 0)$ has (3,1)-steps energy penalty and the zeros distribution shows only single arc approaching real axis. The $\chi = (4, 3, 0)$ in Figure 8 has (1,3)-steps energy penalty and it shows two lines approaching the real axis. Looking at their energy steps, these two cases are inverse to each other.

By referring to Figure 9 for the inverse zeros case $\chi = e^{-\beta J}$, the ferromagnetic region is now in $[0, 1]$ region and the $[1, \infty)$ is the antiferromagnetic region. The ferromagnetic region of $\chi = (4, 3, 0)$ corresponds to the antiferromagnetic region of $\chi = (4, 1, 0)$. The previous examples between $\chi = (3, 1, 0)$ and $\chi = (3, 2, 0)$ also give the same zeros behaviour and their number of transitions are opposite to each other. The distribution lines are more obvious when we check for the inverse values.

With all the presented zeros distributions, the number of arcs or lines of zeros in the ferromagnetic region are corresponded to the number of the phase transition in the physical system as suggested by Martin [1].

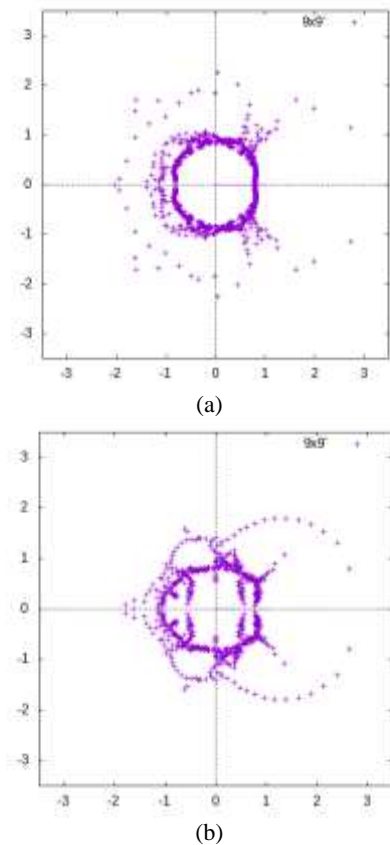


Figure 9 Zeros distribution for $N=9$, $\chi = e^{-\beta J}$; a) $\chi = (4, 1, 0)$, b) $\chi = (4, 3, 0)$.

Here, we also observed that the energy penalty is affected the zeros distribution. The cases with big energy penalty may prefer to have single transition. From our findings, the small energy penalty case has a higher chance for multiple phase transitions than the bigger penalty. Further investigation has to be made for different kind of energy list χ . We will study this separately.

Specific heat

Our finding on the zeros distribution should be in accordance to the physical equation related to phase transition. The existence of the phase transition at the thermodynamic limit is observed when the equation of specific heat has discontinuity. At thermodynamic limit, the graph of specific heat [4] is discontinuous at β_c which gives the critical temperature T_c of phase transition. Detail explanation on specific heat and other functions of states are in [1, 4, 5].

From the classical thermodynamic relation, Helmholtz free energy is defined as

$$F = \langle U \rangle - TS \quad (10)$$

where $\langle U \rangle$ is an internal energy, T is temperature, and S is an entropy [5, 17]. This relation is equivalent to the logarithm of partition function given by

$$F = -k_B T \ln(Z). \quad (11)$$

From the free energy, the second derivative of logarithm of the partition function gives the definition of the specific heat C_v with respect to β as

$$\frac{C_v}{k_B} = -\beta^2 \frac{d^2 \ln Z}{d\beta^2} = \beta^2 \frac{d}{d\beta} U(\beta) \quad (12)$$

where $U(\beta)$ is the internal energy and the first derivative of the logarithm of the partition function.

Here, we continue with the specific heat graph of the Z_5 -symmetric model for some values of χ . From this plot, the peak becomes sharper as the lattice size increases. At thermodynamic limit, this peak is expected to have discontinuity by showing the exact critical point of phase transition. Interestingly for finite size, this behaviour is already observed. To support our observation in the multiplicity of linear arc in the zeros distribution, we plot the graph of specific heat in this section.

Figure 10(a) shows the graph of the specific heat for Z_5 -symmetric model with three different energy levels, $\chi = (2,1,0)$, $\chi = (3,1,0)$ and $\chi = (3,2,0)$. Distinct peak behaviors are shown in the graph. For $\chi = (2,1,0)$ and $\chi = (3,1,0)$, there is only single peak which indicates one phase transition. Whereas, for the $\chi = (3,2,0)$, there are two peaks suggesting for two phase transitions. We have two peaks for the case with two lines in physical region.

The peak behaviors of the graph for $\chi = (3,2,0)$ for increasing lattice sizes $N = 7, 8, 9$ are presented in Figure 10(b). As size increases, the peak becomes steeper.

We claimed that the number of peak is in accordance to the prediction of the number of phase transition through the existence of a particular single arc or multiple arcs in the graph of zeros distribution. This finding supports the existence of the multiple transition points in this model.

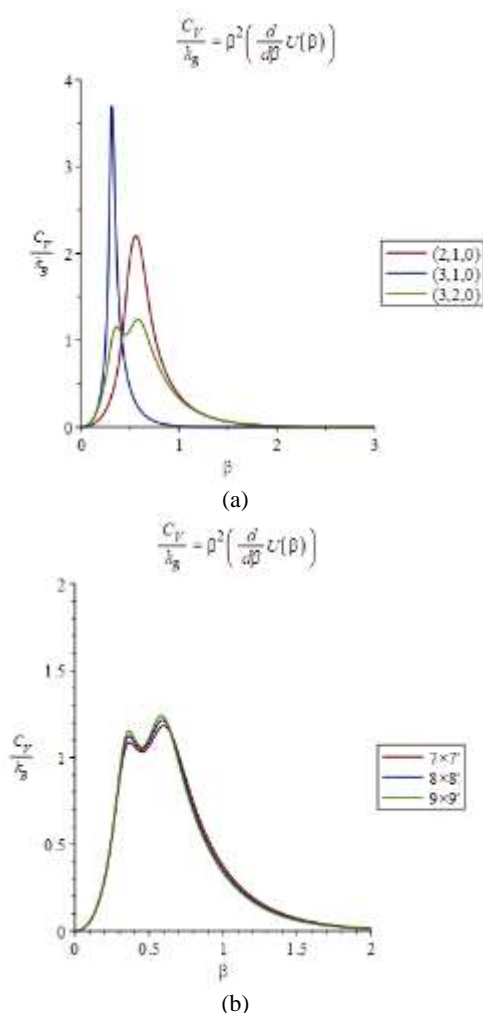


Figure 10 Graph of specific heat C_V for (a) $9 \times 9'$ with different χ and (b) $7 \times 7'$, $8 \times 8'$, $9 \times 9'$ for $\chi = (3, 2, 0)$.

CONCLUSION

We have studied the partition function and its zeros for Z_5 -symmetric models on triangular lattices. This study extends the work by Martin [1] and Zakaria [16] on square lattices. The zeros are plotted in the complex Argand plane in order to study their distributions. From the obtained results, we can see that there are multiple phase transitions based on the number of arcs in the graph and this finding is

supported through the observation from the peak in the specific heat graph. This result is an added evidence to the capability of this model to determine the existence of the multiple phase transitions illustratively. Note that the study of zeros is important because we can study other aspects of phase transition, especially just before the occurrence of the phase transition as mentioned by [12] for square lattice – other lattice types will be discussed elsewhere. Our study is limited by the computing resources, so the zeros distribution can be extended to other larger lattice sizes as well as on different types of lattices and boundary conditions in the future – subject to the advancement of computing technology.

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REFERENCES

- [1] P. Martin, *Potts Models And Related Problems In Statistical Mechanics*. World Scientific Publishing Company, 1991.
- [2] E. Ising, Beitrag zur Theorie des Ferromagnetismus, *Zeitschrift für Phys.*, vol. 31, no. 1, pp. 253–258, Feb. 1925.
- [3] R. J. Baxter F. R. S., H. Brace Jovanovich, P. London San Diego New York Berkeley Boston Sydney Tokyo Toronto, *Exactly Solved Models in Statistical Mechanics*. Academic Press, 1982.
- [4] J. M. Yeomans, *Statistical Mechanics of Phase Transitions*. Clarendon Press, 1992.
- [5] K. Huang, *Statistical Mechanics 2nd Edition*. John Wiley & Sons Ltd, p. 493, 1987.
- [6] S. G. Brush, History of the Lenz-Ising model. *Reviews of Modern Physics*, vol. 39, no. 4, pp. 883–893, Oct. 1967.
- [7] L. Onsager, Crystal statistics. I. A two-dimensional model with an order-disorder transition. *Physical Review*, vol. 65, no. 3–4, p. 117, 1944.
- [8] M. E. Fisher, *The Nature of Critical Points*. University of Colorado Press, 1965.
- [9] S. Ono, Y. Karaki, M. Suzuki, C. Kawabata, Statistical mechanics of three-dimensional finite Ising model. *Physics Letters A*, vol. 24, no. 12, pp. 703–704, 1967.
- [10] S. Katsura, Distribution of roots of the partition function in the complex temperature plane. *Progress of Theoretical and Experimental Physics*, vol. 38, no. 6, pp. 1415–1417, 1967.
- [11] R. Abe, Logarithmic singularity of specific heat near the transition point in the Ising model. *Progress of Theoretical and Experimental Physics*, vol. 37, no. 6, pp. 1070–1079, 1967.
- [12] P. P. Martin, S. F. Zakaria, Zeros of the 3-state Potts model partition function for the square lattice revisited. *Journal of Statistical Mechanics: Theory and Experiment*, vol. 2019, no. 8, p. 84003, 2019.
- [13] R. G. Ghulghazaryan, N. S. Ananikian, Partition function zeros of the one-dimensional Potts model: the recursive method. *Journal of Physics A: Mathematical and General*, vol. 36, no. 23, p. 6297, 2003.
- [14] R. H. Swendsen, *An Introduction to Statistical Mechanics and Thermodynamics*. Oxford University Press, 2012.
- [15] T. D. Lee, C. N. Yang, Statistical Theory of equations of state and phase transitions. II. Lattice gas and Ising model. *Physical Review*, vol. 87, no. 3, pp. 410–419, Aug. 1952.
- [16] F. Zakaria, Analytic properties of potts and Ising model partition functions and the relationship between analytic properties and phase transitions in equilibrium statistical mechanics. PhD thesis, University of Leeds, 2016.
- [17] R. Diestel, *Graph Theory*. Springer, 2006.
- [18] A. Papoulis and S. U. Pillai, *Probability, Random Variables, and Stochastic Processes*. McGraw-Hill, 2001.
- [19] C.-N. Chen, C.-K. Hu, and F. Y. Wu, Partition function zeros of the square lattice Potts model. *Physical Review Letters*, vol. 76, no. 2, p. 169, 1996.